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ENERGETICS OF BCC-FCC LATTICE DEFORMATION IN IRON

GENRICH L. KRASKO
U.S. ARMY MATERIALS TECHNOLOGY LABORATORY
METALS RESEARCH BRANCH

GREGORY B. OLSON
NORTHWESTERN UNIVERSITY,
DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, EVANSTON, IL

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*Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208

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ABSTRACT

The lattice deformation of the BCC-FCC martensitic transformation in iron can be described as a continuous change of the c/a parameter of the body-centered tetragonal (BCT) lattice from c/a = 1 (BCC) to c/a = $\sqrt{2}$ (FCC). Along this deformation path, the total energy (as a function of volume), the enthalpy (as a function of pressure), and the pressure-volume relations – both for nonmagnetic (NM) and ferromagnetic (FM) states – were calculated using the *ab initio* LMTO method. The ground-state magnetic properties, ferromagnetic contributions to the total energy and magnetic moments, were found by making use of the Stoner theory of itinerant ferromagnetism rather than spin-polarized calculations. This circumvents the difficulties of using the traditional local spin-density approximation which fails to correctly describe the energetics of iron phases. The Stoner exchange parameter, I, was calculated from the linear response theory for each c/a as a function of volume. Then, a constant enhancement factor, β, was introduced and the new Stoner parameter, βI, was used in all of the calculations. The factor β was found by fitting the equilibrium atomic volume of the FM BCC phase to its experimental value. No other adjustments of any quantities were performed. The calculations revealed a somewhat unusual behavior of enthalpy along the deformation path. Instead of a double-well curve with a barrier maximum somewhere at 1 < c/a < $\sqrt{2}$, the enthalpy of the NM phase exhibits a monotonic decrease with c/a; the BCC modification being unstable with respect to the shear deformation. Moreover, up to a certain c/a (depending on pressure), the nonmagnetic BCT phase is also unstable with respect to spontaneous magnetization. Ferromagnetism stabilizes the BCT phases. However, the FM FCC phase is unstable with respect to shear deformation. The enthalpy curve along the deformation path then has a cusp corresponding to a first-order phase transition between ferromagnetic and nonmagnetic states accompanied by an appreciable volume discontinuity. The bulk modulus, the magnetic moments, and the BCC-FCC enthalpy differences are in good agreement with the available experimental data.

INTRODUCTION

The BCC-FCC phase transformation in iron lies at the core of the unique properties of iron-based materials. This transformation, being a typical representative of the family of martensitic transformations (MT), has been studied for decades, (e.g., References 1 through 5). Unlike most of the polymorphic transformations in solids, the MT is a diffusionless process involving a correlated motion of many atoms. One important aspect of such motion is the energetics of large-strain homogeneous lattice deformation. This contributes a local energy density of importance to interfacial energy and mobility, as well as the energetics of potential nonclassical nucleation mechanisms.[1,2] The homogeneous deformation mechanism allows continuous crystallographic transition from initial to final phase. In the case of the BCC-FCC MT, a few homogeneous strain paths have been suggested (e.g., Reference 5). The simplest one, known as the Bain deformation,[6] consists of a continuous expansion of a BCC lattice along one of the cubic axes with a contraction along the two others. When the c/a ratio reaches the value $\sqrt{2}$, the BCT lattice just becomes FCC. Due to its simplicity, the mechanism is a very convenient tool of investigating the energetics of the transformation. In the past, it has been used in both phenomenological and *ab initio* calculations of the energetics of MT.[*,7-9]

Along the deformation path $1 \leq c/a \leq \sqrt{2}$, one obviously expects the total energy (or the enthalpy in the constant pressure regime) to undergo a maximum. The nature of this maximum in the case of iron is not clear *a priori*. At low temperatures and moderate positive pressures, BCC iron is ferromagnetism while FCC iron is paramagnetic. Somewhere along the transformation path the ferromagnetism is to disappear. One can expect that this magnetic transition plays a major role in the transformation energetics.

So far, no reliable information on the value of the enthalpy maximum or the enthalpy profile as a whole is available. Phenomenological calculations[10] suggest a high enthalpy barrier, but no first principles, microscopic calculations of the total energy (or enthalpy) of iron along the Bain path, has been done thus far. Such calculations are the objective of the present work.

In recent years, iron has been the objective of extensive study by various first principles methods (for references and comparison of results for iron obtained by different methods, see References 11 through 15). However, the self-consistent spin-polarized calculations of BCC iron inevitably failed to predict the relative stability of the FM BCC phase with respect to nonmagnetic FCC (see discussion in Reference 15). This failure is believed to be mainly due to the local spin-density approximation used in the calculations.

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Because of this fundamental difficulty, at the present time, an entirely first principles analysis of the structural phase transformation in iron is obviously impossible. A way out of this deadlock would be to introduce into the theory an adjustable parameter in order to make calculations more consistent with experimental observations.

Along this path, we have chosen to calculate the equilibrium magnetic moments, as well as the magnetic contributions to the ground state energies of iron using the Stoner model of itinerant ferromagnetism,[16] rather than performing spin-polarized calculations. The exchange parameter, I, can then serve as an adjustable parameter. Having made only one adjustment, such a procedure enabled us to perform the complete analysis of the energetics of the BCC-FCC phase transformation in iron.

We used the LMTO method[17-19] with the so-called combined correction term[17-19] and the Madelung electrostatic correction.*,[20,21] Scalar relativistic calculations on uniform meshes of 1540 points in the irreducible wedges of BCT Brillouin zones were done, with the exchange correlation functional of von Barth and Hedin.[22] Also, the frozen core approximation was used.[23]

PROCEDURE OF THE CALCULATIONS

Recently, the Stoner model was extensively used in total energy calculations.[24-26] Particularly, the metamagnetic behavior of FCC iron was analyzed in detail.[24] Also, the structural properties of BCC and FCC iron were calculated.[26] In the latter paper, the procedure of adjusting the Stoner parameter mentioned above was introduced. The idea was to adjust the value of I so that the equilibrium atomic volume Ω (or the Wigner-Seitz radius, s) of the FM BCC phase was equal to the experimental value. Then the Stoner parameter is $I = \beta I_0$, where β is the enhancement factor and I_0 is the Stoner parameter as found from the linear response theory.[27] In Reference 26, it was found that $\beta = 1.075$. This value was used in the present calculations for all the atomic volumes along the Bain path. No other adjustments of any parameters were done. The enhancement of the Stoner parameter is, in fact, just an enhancement of spin-spin correlations, which the local spin density approximation is known to underestimate.

Our calculations were done for 17 c/a points; $0.92 \leq c/a \leq 1.46$. For each c/a, self-consistent nonspin-polarized calculations were performed for nine values of the Wigner-Seitz radius s (2.521 a.u. $\leq$ s $\leq$ 2.788 a.u.). In each calculation, after convergence had been achieved, I_0 (c/a, s), and then I (c/a, s) $= 1.075$ I_0 (c/a, s) were found, the Stoner equation was solved for the equilibrium magnetic moment, m, and magnetic energy E_m was calculated

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(see Equations 1 through 3 of Reference 24). In a metamagnetic situation, all the stable magnetic solutions were identified.

In the next step, the total energy (consisting of the nonmagnetic, magnetic, and electrostatic contributions) was approximated (with rms $\approx$ 0.03 mRy) by the six-term function

$$E \ (c/a, \ s) \ = \ E_1 \ + \ E_2/\Omega^{2/3} \ + \ E_3/\Omega^{4/3} \ + \ E_4/\Omega^{6/3} \ + \ E_5/\Omega^{8/3} \ + \ E_6/\Omega^{10/3}.$$

The pressure, P, and the bulk modulus, B, were then found by analytic differentiation with respect to the atomic volume, Ω.

RESULTS

Energetics of BCC and FCC Phases

We first briefly summarize the results for the BCC and FCC phases of iron (see also Reference 26). Figure 1 shows plots of the total energies and enthalpies of BCC and FCC iron. As one can see, the FM BCC phase has the lowest energy. The NM BCC phase was always believed to be metastable; i.e., having a higher energy, but corresponding to an energy minimum. The unexpected result is, however, that the NM BCC phase is unstable with respect to spontaneous magnetization over the entire range of the volumes considered. This is the direct consequence of the fact that the density of states at the Fermi level of NM BCC iron is too high for a nonspin-polarized solution to exist (one should distinguish the nonmagnetic and paramagnetic states: the latter corresponds to disappearance of the magnetic long-range order, while in the former, any magnetization is absent).
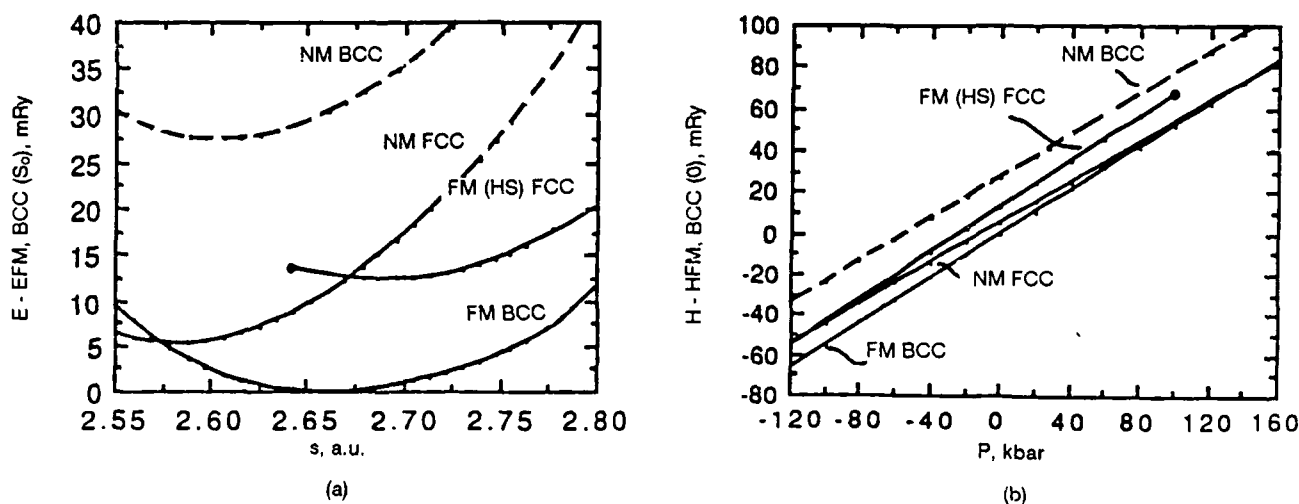
Figure 1. (a) The total energies of BCC and FCC phases versus the Wigner-Seitz radius, s. (b) The enthalpies versus pressure, P. The broken lines here and in Figures 2 and 3 indicate instability with respect to spontaneous magnetization. For the FCC phase, only the high spin FM solution is shown. The bold dots here and in Figure 3 mark the points where the FM solution disappears.

As was shown in Reference 24, at a constant volume regime in FCC, three FM states may be stable (metamagnetic situation). The high spin (HS) energy curve shown in Figure 1a demonstrates existence of FM metastable states. Another intersection of energy curves (under compression) corresponds to the FM BCC-NM FCC phase transformation.

3

The corresponding enthalpy plots are shown in Figure 1b. One can see that the FM BCC-NM FCC phase transformation occurs at P = 145 kbar. Empirical calculations[28] give 150 kbar for this point. Experimentally, at 0 K, the FM BCC-NM HCP phase transition would be observed at approximately the same pressure.[28]

Tables 1 and 2 summarize our results for BCC and FCC iron. One can see that having made only one adjustment, that of the Stoner parameter, the theory gives the equilibrium Wigner-Seitz radii, s_0, the bulk moduli, B, the magnetic moments, m, and the BCC-FCC enthalpy difference at P = O in excellent agreement with experiment.

Table 1. COMPARISON OF CALCULATED AND EXPERIMENTAL
STRUCTURAL PROPERTIES OF BCC AND FCC IRON

	FM BCC		NM FCC		FM FCC*	
	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.
s_0 (a.u.)	2.659	2.661†	2.588	2.62‡	2.690	2.68**
B (Mbar)	1.689	1.67#	3.122		2.317	
m (μ_B/at)	2.223	2.15##			2.595	2.4 - 2.8**

*HS
†Reference 29
‡Empirical calc., Reference 28
**Two spin model, Reference 28
#Reference 30
##Reference 11

Table 2. BCC-FCC ENTHALPY DIFFERENCE AT P = 0

	$E_{NM\ FCC}$ - $E_{FM\ BCC}$		
	Calc.	Exp.	
mRY/atom	5.307	4.166*	3.692†
(cal/mole)	(1659)	(1303)	(1155)

*Reference 28
†Reference 31

Along the Bain Path

From an intuitive point of view, one could expect that upon imposing a uniform deformation, the enthalpy plots of both NM and FM phases would have two-well shapes with minima at the BCC and FCC states and a smooth maximum at $1 \leq c/a \leq \sqrt{2}$. Unexpectedly, the calculated picture is quite different.

28 KAUFMAN, L., and BERNSTEIN, H. Computer Calculations of Phase Diagrams. Academic Press, New York, 1970.
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Figure 2 shows our results for three pressures: 140, 0, and -120 kbar. At 140 kbar, the FM BCC and NM FCC phases are almost at equilibrium (the exact equilibrium takes place at 145 kbar, as one can see from Figure 1b). Though we already know that the NM BCC phase is unstable with respect to spontaneous magnetization, we still could expect that, disregarding the magnetic instability, it corresponds to an enthalpy minimum along the c/a path. One can see, however, that the NM BCC enthalpies have maxima; e.g., the NM BCC phase is also unstable with respect to infinitesimal tetragonal (shear) deformation.

(a)

(b)

(c)
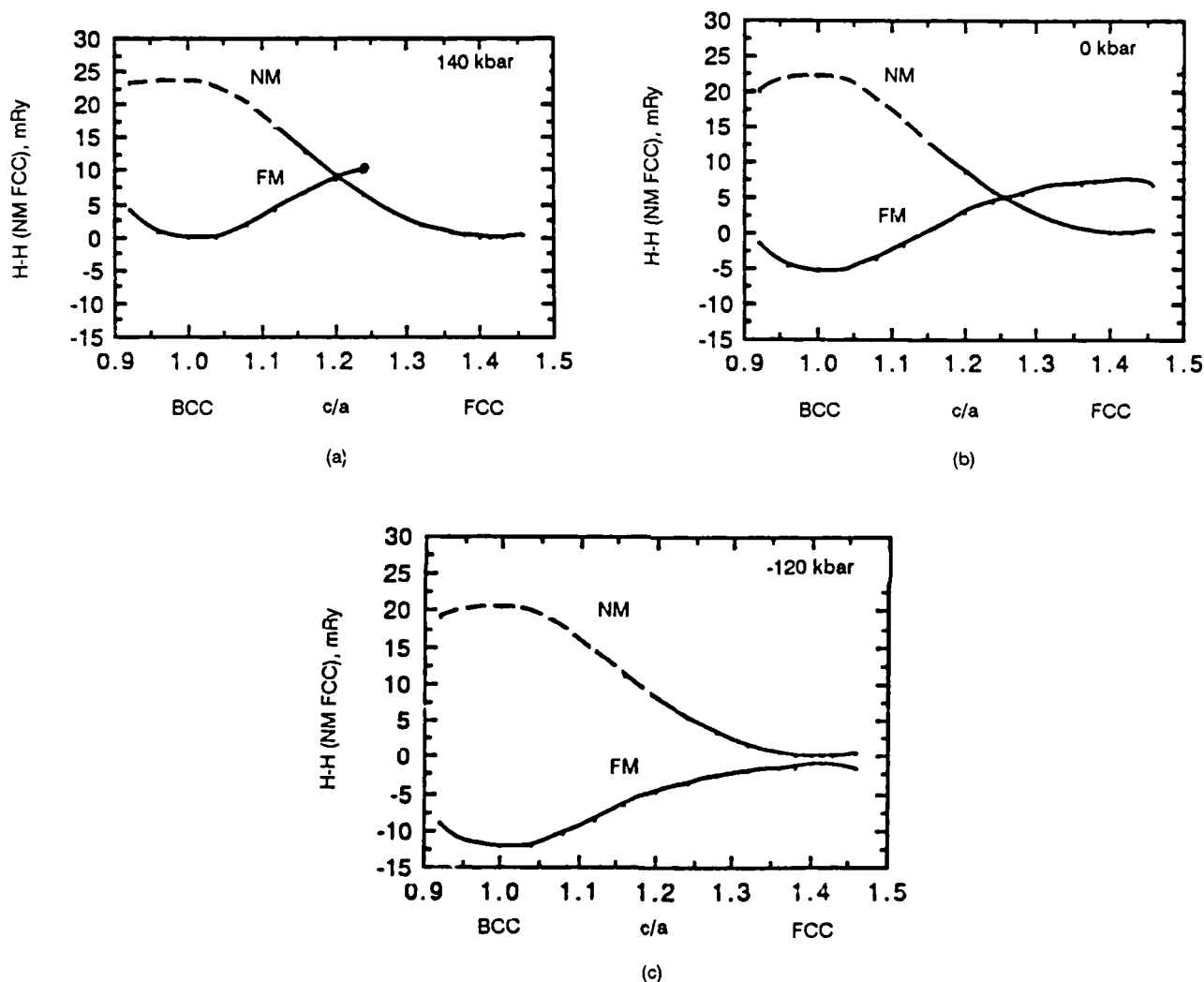
Figure 2. The enthalpy plots along the Bain path for three pressures.

The FM contribution stabilizes the BCT phases. The enthalpy of FM BCT has a minimum at c/a = 1. However, at high pressures approaching the FCC point, ferromagnetism disappears; the FM solution does not correspond to an extremum (neither a minimum or maximum) of energy (or enthalpy). At lower pressures, however, where the FM solution does exist, the FM FCC phase corresponds to an enthalpy maximum. This simply means that the FM FCC phase is unstable with respect to infinitesimal tetragonal deformation and, therefore, cannot exist.

This is an important new result. In the past, in order to explain the thermodynamics of FCC iron, a two-spin model was postulated.[28,32,33] It was suggested that two magnetic states, high spin FM and low spin antiferromagnetic (AFM), could exist in FCC iron. We have found, however, that a FM state in FCC iron is unstable; an AFM state can exist and, in fact, is observed experimentally at low temperatures.[34,35] As for the FM FCC phase, it was observed as precipitates in Cu-Au alloys.[36] Also, thin FCC films grown epitaxially on Cu surfaces were also reported to be FM.[37,38] In both cases, finite size effects could be responsible for the relative stability of the FM BCC phase.

Thus, going along the Bain path from BCC to FCC, first the FM BCC phase is stable, but around c/a = 1.2, a first-order phase transition occurs and, at higher c/a, the NM FCC phase is stable. As a result, the enthalpy plot is not a smooth two-well curve, but has a cusp.

The shown plots for the three pressures have common features. As a matter of fact, the FM and NM curves are almost identical for the three pressures, but shifted with respect to each other. Upon lowering the pressure, the intersection point (and the cusp) shift to the FCC direction, and the FM phase has a greater area of stability. At about -110 kbar, the NM FCC is no longer stable. Sitting in the FCC point, one can see that the FM state has the lower energy, which looks like a FM-NM phase transition (Figures 1a and 1b). However, as discussed above, the FM FCC is unstable with respect to the infinitesimal tetragonal deformation. As a result, with such an expansion, the FCC phase ceases to exist (however, we do not know how an AFM phase would behave at such a negative pressure).

The FM phases always have higher volumes compared to their NM counterparts. Therefore, the first-order phase transitions along the Bain path are accompanied by a considerable volume discontinuity at the cusp points. Figure 3 shows the plots of atomic volume versus c/a for P = 0 kbar. The arrow indicates the discontinuity in volume at the cusp point, which is quite big – almost 10%.
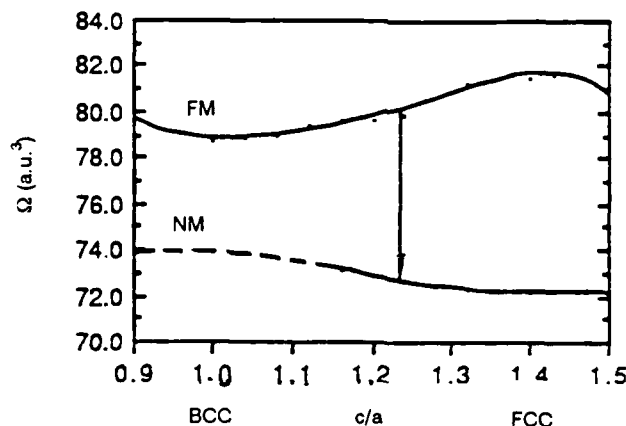
Figure 3. Atomic volume versus c/a for P = 0 kbar.
The arrow shows discontinuity at the cusp point.

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CONCLUSIONS

Using the Stoner model with the adjusted exchange parameter, we have calculated, for the first time, the structural properties of BCC and FCC iron and the energetics of the intermediate states along the Bain deformation path. Unexpected and somewhat unusual features of the energetics were discovered. For the first time, it is shown that the NM BCC phase cannot exist due to magnetic and shear instabilities. Another important result is that the FM FCC phase is also unstable with respect to tetragonal deformation. The suggested approach paves the way for "first principles" detailed studies of the behavior of iron and iron-based systems. Among the problems of interest is the energetics of grain boundaries. LMTO supercell calculations of a grain boundary with and without impurity atoms are currently in progress. Another problem which can be addressed using the developed approach is the calculation of the energetics of coherent interface boundaries of importance to nucleation processes. In the case of the BCC-FCC martensitic transformation, the latter may involve orthorhombic, rather than tetragonal distortions. Theoretical study of such problems may provide an important contribution to the quantitative control of transformation kinetics.

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2   Authors

U.S. Army Materials Technology Laboratory
Watertown, Massachusetts 02172-0001
ENERGETICS OF BCC-FCC LATTICE
DEFORMATION IN IRON -
Genrich L. Krasko and Gregory B. Olson

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The lattice deformation of the BCC-FCC martensitic transformation in iron can be described as a continuous change of the c/a parameter of the body-centered tetragonal (BCT) lattice from $c/a = 1$ (BCC) to $c/a = \sqrt{2}$ (FCC). Along this deformation path, the total energy (as a function of volume), the enthalpy (as a function of pressure), and the pressure-volume relations – both for nonmagnetic (NM) and ferromagnetic (FM) states – were calculated using the ab initio LMTO method. The ground-state magnetic properties, ferromagnetic contributions to the total energy and magnetic moments, were found by making use of the Stoner theory of itinerant ferromagnetism rather than spin-polarized calculations. This circumvents the difficulties of using the traditional local spin-density approximation which fails to correctly describe the energetics of iron phases. The Stoner exchange parameter, I, was calculated from the linear response theory for each c/a as a function of volume. Then, a constant enhancement factor, β, was introduced and the new Stoner parameter, βI, was used in all of the calculations. The factor β was found by fitting the equilibrium atomic volume of the FM BCC phase to its experimental value. No other adjustments of any quantities were performed. The calculations revealed a somewhat unusual behavior of enthalpy along the deformation path. Instead of a double-well curve with a barrier maximum somewhere at $1 < c/a < \sqrt{2}$, the enthalpy of the NM phase exhibits a monotonic decrease with c/a; the BCC modification being unstable with respect to the shear deformation. Moreover, up to a certain c/a (depending on pressure), the nonmagnetic BCT phase is also unstable with respect to spontaneous magnetization. Ferromagnetism stabilizes the BCT phases. However, the FM FCC phase is unstable with respect to shear deformation. The enthalpy curve along the deformation path then has a cusp corresponding to a first-order phase transition between ferromagnetic and nonmagnetic states accompanied by an appreciable volume discontinuity. The bulk modulus, the magnetic moments, and the BCC-FCC enthalpy differences are in good agreement with the available experimental data.